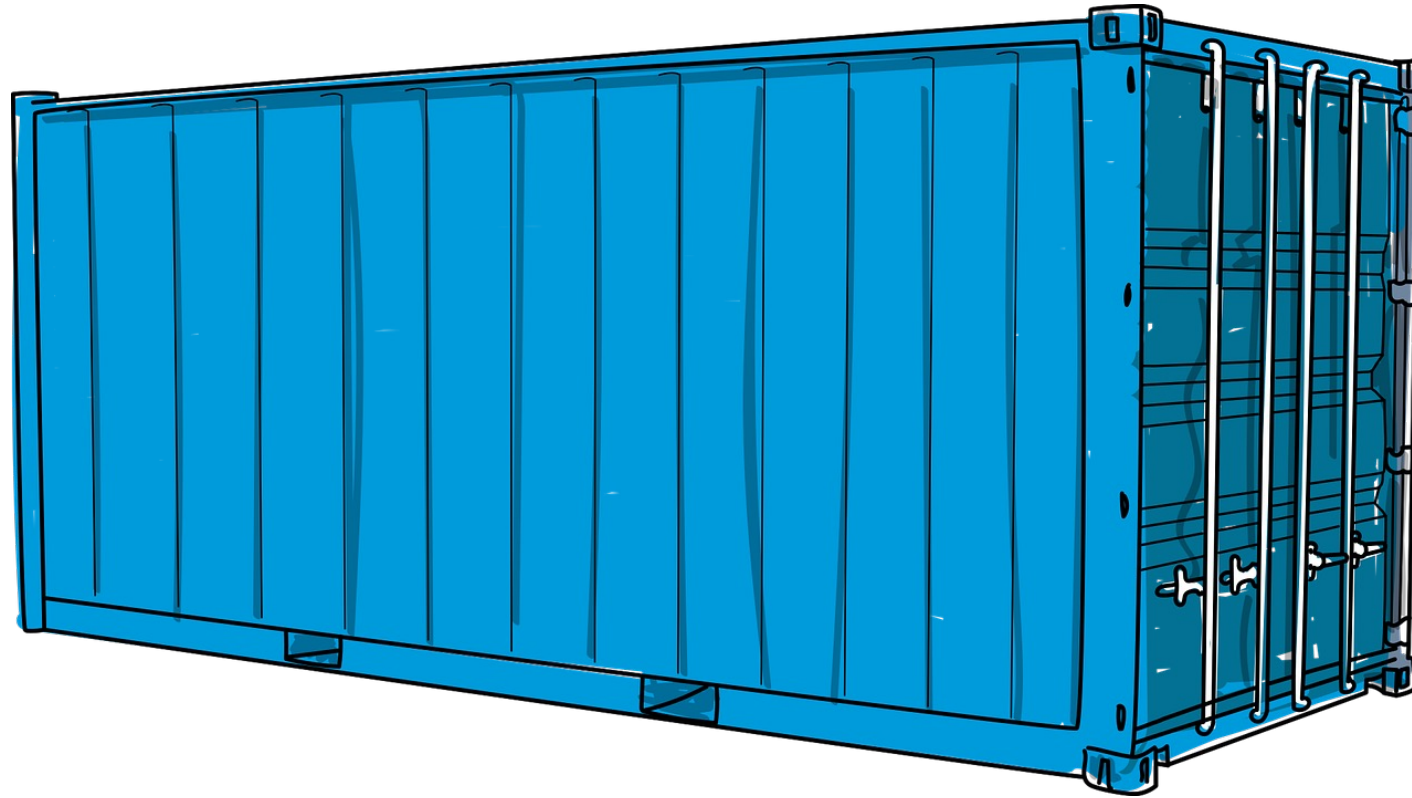# HPC series
Containers

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Containers in HPC

Intro to HPC containers

What are containers ?

- **Containers** pack an application/workflow/pipeline and all of its dependencies into a single image [HLSU2021].

Why use containers ?

- Can't install software because of unavailable system dependency like libssl-dev, glibc, libopenssl-devel...

- Need to install new software/libraries on old OS platforms

- Need reproducibility of a complex software compilation
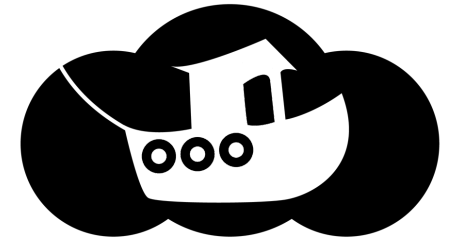
Container technologies
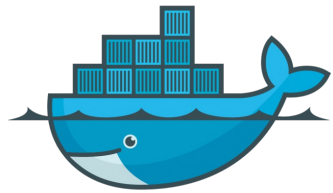
Designed for system services/software development

Docker needs root, podman no

Very large user community

Docker Hub: huge depo of ready-to-use containers

Specifically designed for HPC

Don't need root access

Singularity/Apptainer most widely used container system for HPC [APTN2023]

Can make use of Docker Hub

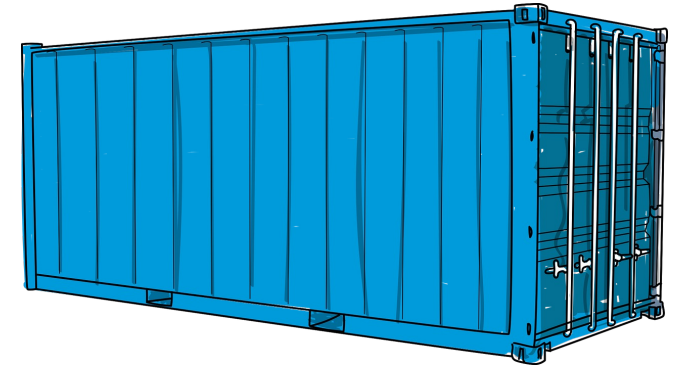# How to build a container

Recipe

soft-ver.def

build →

Image

soft-ver.sif

run →

Container

How to build a container

1. Create singularity recipe "samltools-1.3.def":

```
vi samtools-1.3.def
```

```
BootStrap: docker
From: debian:10

%environment
    export LC_ALL=C

%post
    apt -y update && apt -y install wget zlib1g zlib1g-dev bzip2 build-essential libncurses5-dev
    wget https://github.com/samtools/samtools/releases/download/1.3/samtools-1.3.tar.bz2
    tar -xjf samtools-1.3.tar.bz2
    cd samtools-1.3 && ./configure &&  make && make install
    mkdir -p /data/user
```

✈Tip: use "singularity help build" on how to write a .def file.

How to build a container

2. Build image "samtools-1.3.sif " using above recipe:

```
singularity build samtools-1.3.sif samtools-1.3.def
```

3. Run your container:

```
singularity run samtools-1.3.sif
```

4. Use your container with SBATCH

Building image from sandbox

When building a recipe (.def) from scratch, you can build a base sandbox from any DEF FILE BASE OS, make changes to it, then build sif:

```
singularity build --sandbox /tmp/debian
docker://debian:latest
singularity exec --writable /tmp/debian apt-get
install python
singularity build /tmp/debian2.sif /tmp/debian
```

Practice

Pick a bioinfo software of your choice and follow above intructions to build a container for it.

References

Web references:

- [HLSU2021]   Introduction to Singularity retrieved from http://www.hpc.lsu.edu/training/weekly-materials/2021-Spring/HPC_Singularity_Spring2021.pdf on 28.08.2023

- [APTN2023]   Apptainer website https://apptainer.org consulted on 28.08.2023